Glutaric acid, 2-(2-fluorophenyl)ethyl undecyl ester

Inchi: InChI=1S/C24H37FO4/c1-2-3-4-5-6-7-8-9-12-19-28-23(26)16-13-17-24(27)29-20-18-21-1
InchiKey: ZQMUBGFJGQCWDR-UHFFFAOYSA-N
Formula: C24H37FO4
SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1F
Mol. weight [g/mol]: 408.55

Physical Properties

Property code	Value	Unit	Source
gf	-408.67	kJ/mol	Joback Method
hf	-999.34	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	89.45	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.156		Crippen Method
mcvol	341.910	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	2902.00		NIST Webbook
rinpol	2902.00		NIST Webbook
tb	932.03	K	Joback Method
tc	1141.08	K	Joback Method
tf	544.09	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.42	J/mol×K	932.03	Joback Method
cpg	1143.28	J/mol×K	966.87	Joback Method
cpg	1158.79	J/mol×K	1001.71	Joback Method
cpg	1172.97	J/mol×K	1036.55	Joback Method
cpg	1185.87	J/mol×K	1071.39	Joback Method
cpg	1197.53	J/mol×K	1106.24	Joback Method
cpg	1207.99	J/mol×K	1141.08	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume